“Simulation method for thermoelectric transport in complex bandstructure bipolar materials”

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We present a computational method to compute the transport coefficients in bipolar complex bandstructure materials. We couple the Boltzmann transport method within the energy and momentum dependent relaxation time approximation to DFT bands for half-Heusler materials, considering both electron-phonon and ionized dopant scattering. The full energy and momentum dependence of the relaxation times is essential in capturing the correct transport features. We then compare the conventional combination of unipolar transport coefficients with the simultaneous consideration of the full bipolar effects in the calculation of the transport coefficients. A large difference between the two treatments exists for narrow bandgap materials.

Lightly doped narrow gap semiconductors with asymmetric conduction/valence bands offer the unconventional possibility to achieve extremely high thermoelectric power factors of up to 50 mW/mK^2, if they possess highly asymmetric conduction and valence bands in terms of density of states or phonon scattering rates. This is achieved because, under these conditions, charge transport becomes phonon scattering-limited, which allows large conductivities. Finally, we interpret related experimental findings.

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